Supporting Information

Profoundly improved photostability of dimetronidazole by cocrystallization

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Table S1. Intermolecular interaction energies estimated using CE-B3LYP dispersion-corrected DFT models. Both the total energy ($E_{(tot)}$) and electrostatic ($E_{(ele)}$), polarization ($E_{(pol)}$), dispersion ($E_{(dis)}$), and exchange-repulsion ($E_{(rep)}$) components are listed (kJ/mol). R indicated the distance between centers of mass of the pair of molecules (Å).

DMZ-SAC

N	Symop	R	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
1	-	7.23	-11.6	-2.9	-8.3	9.5	-15.9
1	-	6.92	4	-2.6	-11.4	9	-2.1
1	-x, -y, -z	8.87	-0.8	-0.5	-4.5	1.2	-4.4
1	-	3.78	-5	-2.9	-43.5	27.4	-28.4
1	-	8.58	-11.5	-2.5	-8	9.1	-15.3
1	-	7.28	-14.1	-3.2	-8.3	13.8	-16
1	-	8.8	-6.9	-2.1	-6.9	9.2	-9.2
2	x, y, z	7.99	-2.8	-0.8	-3.7	0.5	-6.5

2	-x+1/2, y+1/2, -z+1/2	7.12	-2.6	-1.7	-6.3	3.8	-7.2
1	-x, -y, -z	9.09	-1	-0.5	-3.7	0.7	-4.2
1	-	6.61	-74.6	-18.3	-15.4	90.1	-50.2
1	-	3.87	-6.8	-3	-44.6	29.3	-30.2
1	-x, -y, -z	6.73	4.8	-0.6	-7.1	0.8	-1.1
2	x, y, z	7.99	-7.4	-1.8	-7.5	4.6	-12.8
2	-x+1/2, y+1/2, -z+1/2	8.17	-0.1	-1.4	-7.4	2.3	-6.1
1	-x, -y, -z	6.53	7.8	-0.4	-6.8	0.6	2.4
1	-x, -y, -z	6.73	4.8	-0.6	-7.1	0.8	-1.1

DMZ anhydrate

N	Symop	R	E_{ele}	E_{pol}	E_{dis}	E_{rep}	E_{tot}
2	-x, -y, -z	3.76	-10.7	-2	-37.4	20.9	-32.4
4	x+1/2, y+1/2, -z+1/2	6.74	-1.9	-1.7	-9	5.1	-8
2	-x+1/2, -y+1/2, z+1/2	7.39	-15.4	-4.8	-13.2	15.2	-21.9
2	x, y, z	9.15	-6.2	-1.3	-3.6	2.6	-9.1
2	-x+1/2, -y+1/2, z+1/2	6.90	-12.4	-2.4	-7.4	8.9	-15.8

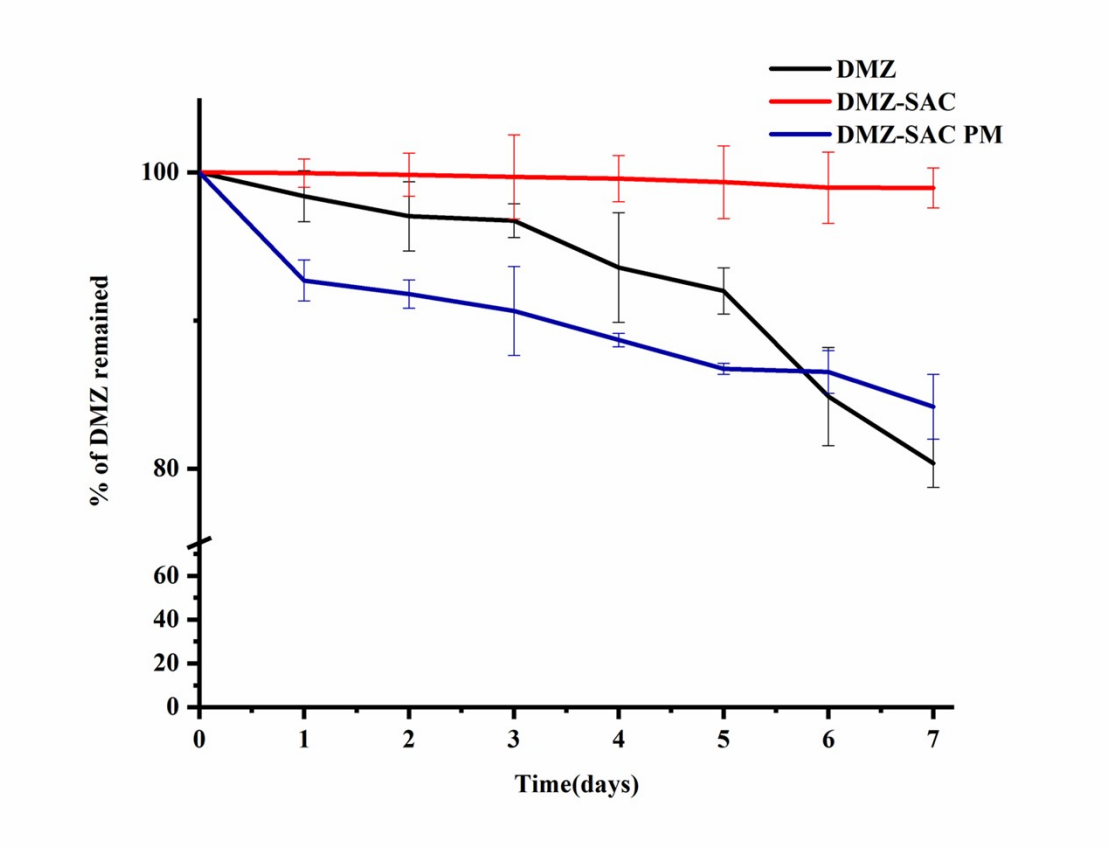

Fig. S1. Comparison of DMZ assay values for pure DMZ powder, physical mixture of DMZ and SAC

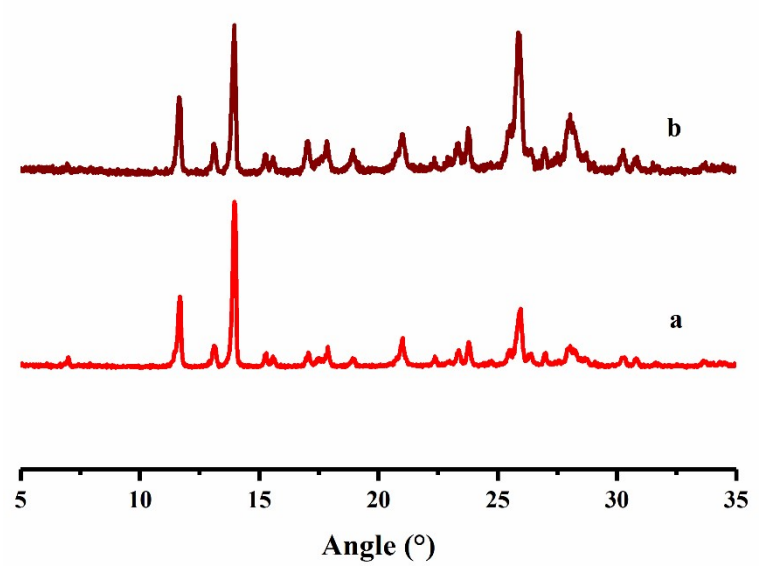

Fig. S2. PXRD patterns of DMZ-SAC (a) before and (b) after powder dissolution experiment